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LLNL-CONF-406899

Hierarchical Material Models for Modeling Fragmentation of Targets in Inertial Confinement Fusion Reseach

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September 10, 2008

International Symposium on Structures Under Earthquake Impact and Blast Loading 2008
Osaka, Japan
October 10, 2008 through October 11, 2008

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HIERARCHICAL MATERIAL MODELS FOR MODELING FRAGMENTATION OF TARGETS IN INERTIAL CONFINEMENT FUSION RESEARCH

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***Keywords*:** Fragmentation, multi-scale simulations, multi-physics

SUMMARY

Fragmentation is a fundamental process that naturally spans the micro to macroscopic scales. Recent advances in algorithms, computer simulations, and hardware enable us to connect the continuum to microstructural regimes in a real simulation through a heterogeneous multiscale mathematical model. Arbitrary Lagrangian Eulerian (ALE) methods are combined with automatic mesh refinement (AMR) in the ALE-AMR code that is the software foundation of the current research. In this talk, we focus on the hierarchical material model (HMM) used to span the material response from the microscale, where fracture and fragmentation are initiated, to the macroscale of the target system. This model is used to predict the response of the target assemblies in the high-powered laser target chambers so that they can be designed to protect the optics and instrumentation from damage. Unlike most physics analyses, which model only the target, the present analyses must include the target shields and pinhole camera arrays, often the source of most of the fragments.

1. INTRODUCTION

Inertial confined fusion (ICF) is one of the most promising approaches to the development of fusion power. Conceptually, it is relatively simple: a large number of laser beams strike a target (either directly or indirectly by the production of x-rays), generate a series of strong shockwaves within it that compresses the target to the point where fusion can occur, and the target's own mass confines it long enough that the energy released by fusion exceeds the energy required by the laser beams. Like many simple ideas, it is very difficult to implement. Large ICF research facilities include the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory and the Laser MegaJoule (LMJ) facility being built by Commissariat à l'énergie atomique or CEA, the French Atomic Energy Commission. In Japan, the GEKKO XII-HIPER (High Intensity Plasma Experimental Research) System is devoted to studying targets in a flexible configuration.

The ICF target is held in the chamber by a support structure and is surrounded by instrumentation. While the lasers completely vaporize the main hohlraum for the case of an indirect-drive target, some of the surrounding diagnostics and other pieces attached to the hohlraum may fragment, sending debris into the instrumentation and laser optics. If the debris is large enough and has enough velocity, the resulting damage may be very expensive in terms of both time and money. Accurately predicting if and how a structure may fragment is therefore a critical part of the design of new experiments.

2. HIGH-POWER LASER FACILITY REQUIREMENTS

The environment of a high-powered laser chamber contains a good deal of open space from the vacuum that surrounds the small fusion target located at the chamber center. One goal of our simulations is to model how the target dismantles after being hit by either laser beams or by x-rays that result from the lasers interacting with other target components. For the purposes of our simulation the "target" includes not only the hohlraum (indirect drive) where the laser is focused, but also ancillary target elements such as cooling rings, shields, or appendages that improve diagnostic capabilities. Pieces of the target that are closest to target center where the laser is focused will be vaporized and thus are relatively benign. However target components that are further from the main laser focus point are subject to lower levels of energy and therefore may be fragmented. It is important to determine the size of these fragmented pieces and their velocity vectors after the laser shot so that optics and diagnostics that line the chamber will be protected from damage. Dedicated experiments as well as experience from recent high-powered laser shots provide information on this environment and the usefulness of mitigation procedures to direct fragments in benign directions [Eder, 2008].

3. ALE METHODS

Solids, liquids, gases, and plasmas must be accurately handled in the simulation. Solid materials are typically modeled using a Lagrangian approach, where the computational mesh deforms with the material. This approach provides the most accurate strain calculations, which are critical for modeling the response of the material, and material interfaces are exactly resolved. If the deformation of the computational mesh is too large, however, the accuracy is degraded and a Lagrangian calculation may go unstable.

Liquids, gases, and plasmas typically undergo very large deformations, and therefore they are simulated using an Eulerian formulation, where the mesh is fixed in space and the material flows through the mesh. An Eulerian formulation is typically more expensive than a Lagrangian formulation because of the transport terms.

Arbitrary Lagrangian Eulerian (ALE) methods allow the mesh to move relative to the material with an arbitrary velocity. If the mesh velocity is the same as the material velocity, the Lagrangian formulation is recovered, and if the mesh velocity is zero, the Eulerian formulation is recovered. ALE methods locally control the mesh velocity to maximize the accuracy and stability of the solution.

There are two types of ALE formulations: 1) simplified ALE methods, and 2) multi-material ALE methods. Simplified ALE (SALE) methods permit only a single material within a finite element, which simplifies the formulation, but restricts the boundaries to be Lagrangian. The restriction on the boundaries limits their usefulness. Multi-material ALE (MMALE) methods allow a single element to contain several materials. This generality allows material boundaries to run through the elements, greatly increasing the robustness of the calculation, and allows for the dynamic creation of new free surfaces through failure, a capability that is necessary for modeling fragmentation accurately.

3.1 Global Computational Strategy

ALE methods are implemented, via operator splitting, as a sequence of three steps.

The first step is the Lagrangian step, and it incrementally updates the material motion for all phases (from solid through plasma) using the central difference method for time integration.

The second step adjusts the motion of the mesh to achieve the best accuracy and stability for the solution. There is no unique methodology for performing this step, and most codes have a range of strategies that the user may try [Benson, 1992].

The last step is the Eulerian, or remap, step. It projects the solution from the original mesh in the first step to the updated mesh of the second step. In most MMALE calculations, it is the most expensive part of the analysis. The solution variables within an element (stress, density, energy, etc) are regarded as piecewise constant during the Lagrangian step. Projecting the piecewise constant solution results in the first order accurate *donor cell advection* method, which is not adequate for large-scale calculations. Modern projection methods, such as MUSCL and WENO, reconstruct higher order polynomial approximations of the solution from the piecewise constant Lagrangian solution, and project them on to the new mesh, yielding second order accurate or better solutions.

3.2 Multi-material Complications

Multi-material formulations have two complications not faced by formulations for a single material. When an element contains more than one material, the contents of an element are described by the volume fractions of its constituent materials, where the volume fraction is simply the ratio of the volume of a particular material and the element volume.

During the Lagrangian step, the incremental deformation of the element must be partitioned between the materials contained by the element. For example, consider an element containing steel and air. If the element is compressed in the direction normal to the interface between the steel and the air, we expect that the compression will be taken up entirely

by the air and the increase in the pressure will be small. On the other hand, if the element is compressed in a direction parallel to the interface, we expect that the deformation will be shared between the air and the steel, and the pressure will increase approximately by the bulk modulus of the steel times its volume fraction of the element times the overall element volume change. The behavior of an element therefore clearly depends on how the materials are distributed within the element and how the element is deformed. The algorithm that calculates this behavior is called the *mixture theory*.

The locations of the material interfaces are required during both the Lagrangian and Eulerian steps. Several strategies for tracking or reconstructing material interfaces have been tried over the years for MMALE methods. The one used here, a *volume of fluid* (VOF) method, has the advantage that the material interfaces are reconstructed every time step so that new free surfaces evolve automatically and naturally as materials fracture, a quality that is critical to modeling fragmentation. These methods cannot be described here due to space limitations, and the interested reader is referred to [Benson, 2002].

4. AUTOMATIC MESH REFINEMENT

The computational mesh governs the accuracy and cost of the analysis: The solution error is proportional to the square of the element size, while the size of the stable time step is inversely proportional to the smallest element in the calculation, and the cost per time step is proportional to the total number of elements. For example, to uniformly reduce the error in the solution by a factor of 4, the number of elements must be increased by a factor of 2 in each direction, and the time step size reset to ½ it previous value, increasing the total cost of the analysis by a factor of $2^3/(1/2)=16$.

The computational mesh must therefore be controlled so that the total number of elements is minimized while guaranteeing that adequate mesh resolution is maintained in the interesting parts of the solution. With the strong shocks traveling across the solution domain and dynamically evolving material interfaces due to material failure, the interesting parts of the solution change their position with time, and it isn't possible to use a single fixed mesh that is both efficient and accurate for the entire duration of the analysis. Automatic (or Adaptive) Mesh Refinement (AMR) automatically refines the mesh where the solution is becoming interesting, and coarsens it where nothing is happening, to maximize the accuracy of the solution while minimizing its cost.

AMR algorithms are too complicated to describe in detail due to space limitations. Their structure, however, can be summarized. First, the regions that require mesh refinement or coarsening are identified by an error indicator, which assigns a value to each element bases on its estimated accuracy in the future. This estimate is often based on estimates of the current accuracy, but it may also anticipate future needs by detecting changes to the solution (e.g., the chemical reaction rate has suddenly increased) that indicate the current mesh will soon be inadequate. Second, a new mesh is created from the old mesh that is appropriately refined or coarsened based on the error indicator. Last, the solution from the old mesh is projected on to the new mesh. The algorithms for performing the last step are similar to the ones used during the Eulerian step.

5. ALE-AMR

The ALE-AMR code is a new code whose primary purpose has been to model the process by which high-powered laser targets and ancillary structures such as metal shields/pinholes spall and fragment when exposed either to laser light or x-rays. It is currently the primary design tool for assessment of potential damage to optics and diagnostics on the National Ignition Facility (NIF), a high-powered laser facility at LLNL.

The code is designed using a unique combination of mathematical and engineering techniques that allow for insertion of different physics models at different levels. The code retains full material histories, and other processes such as surface tension could be added within the framework.

The code also incorporates a sophisticated interface reconstruction technique that allows us to capture the actual sizes and velocities of liquid droplets and solid fragments that are expelled from targets and other surfaces. Figure 1 shows an ALE-AMR simulation of a thin metal foil (red color) that is energized by x-rays at the left front face. Plasma blows off to the left (the green plume), and spall planes form off the rear surface (on the right). The top half of the figure shows just the density and bottom half shows the moving adaptive mesh with four levels of refinement. Small eddies of plasma can be seen in the top left. Note how the code can calculate spall planes and fragmenting particles as well as plasma.

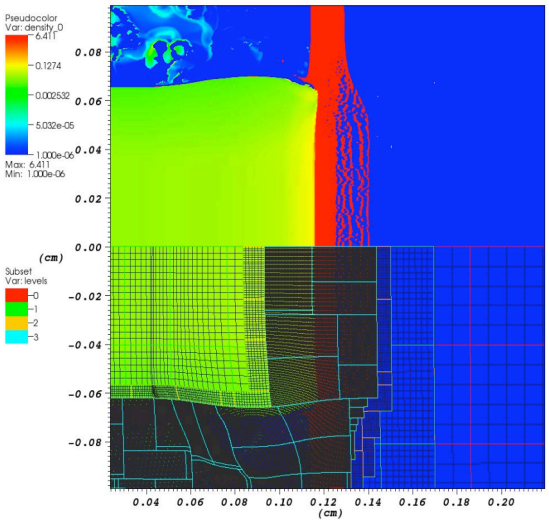

Figure 1: Example simulation using ALE-AMR showing mesh motion and adaptive refinement.

The interface reconstruction scheme in ALE-AMR that allows for droplet formation is implemented in both two and three dimensions. One example of a three dimension problems is given in Figure 2. Here, an aluminum cooling ring of an ICF target breaks into small droplet sized pieces as it is energetically driven from the interior.

AMR with Arbitrary Lagrangian Eulerian Algorithms

Our modeling strategy is built on ALE-AMR algorithms [Anderson, 2004] that are unique in their combination of Lagrangian and ALE techniques [Benson, 1992] with an AMR framework ([Koniges, 2006], [Fisher, 2008], [Masters, 2008]). The majority of ICF codes are normally based on a standard ALE approach. However severe limitations in such simulations that use a fixed number of grid points restrict the use of physics models at different scales. With the ALE-AMR technique, we are able to dynamically drive the multiscale adaptivity through the use of sets of nested grids that automatically coarsen and refine to suit the needs of the simulation. The coarsening and refining is based on a hierarchical grid structure that changes dynamically in time. The software framework supporting this hierarchy is SAMRAI [Gunney, 2006] [Wissink, 2003]. Recent improvements in the scalability of the underlying SAMRAI library show that it scales to 10,000 processors or more.

Referring again to Figure 2, we are able to see the dynamic adaptive mesh. The bottom half of the figure shows the SAMRAI patch boundaries as well as the grid contained in those boundaries. In this simulation, four levels of refinement were used. The code dynamically adds more resolution to areas where it is needed, in this case concentrating the mesh and thus most of the calculation in the area where spall off the back occurs. Note also that the mesh is NOT Eulerian. An Eulerian AMR code would have regular Cartesian patch boundaries. In contrast, the ALE-AMR code includes both the ALE motion and the AMR meshing. So in regions where the mesh distorts to accommodate the expanding plasma plume, the refinement patches also distort.

The SAMRAI library maintains patches or combinations of patches on processors and allows the simulation to achieve a high degree of parallelism. In the proposed work, at the finest level the material models will also be farmed out to processors using the SAMRAI framework. Sophisticated load balancing techniques allow a highly scalable simulation [Koniges, 2008].

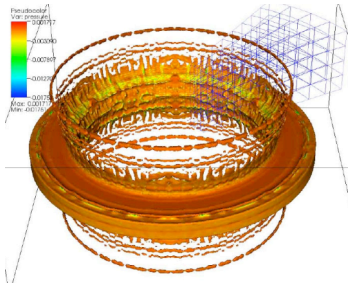

Figure 2. ALE-AMR 3-D application to dynamics of a cooling ring heated from inside.

6. HIERARCHICHAL MATERIAL MODEL

A key objective of the research was the development of hierarchical methods for constructing coarse-grained models at the scales required by the AMR calculation [Fisher, 2008]. Not all aspects of the model described here have been implemented, but we anticipate that the implementation will be completed in the near future. The hierarchical models are based on the concept of nested refinement of a representative volume element (RVE). An RVE is a volume of space containing enough microstructure, e.g. grains, to be well approximated by a continuum model at a certain scale for an illustration of the concept. For convenience, we assume that the RVE is a cube. The relevant RVE is generally much larger than the finest zones used in the subdomain. Assuming that the refinement of a zone consists of subdividing it into n zones on each edge, the RVE is subdivided into n^p of the finest zones on an edge, where p the number of levels in the model. In the figure, there are 3 levels, with each zone at a level subdivided into 9 zones at the next level of refinement.

A Voronoi tessellation is currently used to construct the grains within the RVE, although the method isn't restricted to using it. The boundaries of the grains pass through the zones as indicated in the figure. The first level in the hierarchy of the material model is therefore the single crystal plasticity model of the grain associated with a zone, e.g., the zones within the circle labeled 1 in Figure 3. The second

level is associated with coarsening the finest mesh, the zones within circle 2 in Figure 3. The response of the aggregates at various scales will, in the future, be represented by an innovative interpolation scheme. Instead of working with a yield surface in stress space, the flow stress is interpolated in the deformation rate space and scaled by a viscoplastic rate law similar to the one used in single crystal plasticity. By using this representation, no assumption about the functional form or shape of the yield surface is required and the accuracy of the representation depends only on the resolution of the data used in the interpolation.

The generation of the HMM continues by recursively generating the next level of coarsening from the previous level using the same algorithms used to generate the polycrystalline models. At each level the response is represented by the interpolation scheme, and therefore the memory requirement for any level of coarsening is fixed. This is contrast to faceted representations of the yield surface in stress space that increase in complexity as the number of grains increases.

The RVE tiles the mesh used in the analysis using a parametric coordinate system. Some aspects of the material response at each level of the hierarchy for each subdomain of the RVE will calculated before the analysis so that they are a look-up during the analysis; others will be calculated on-the-fly as described previously by strategies that maximize the information obtained from subscale calculations.

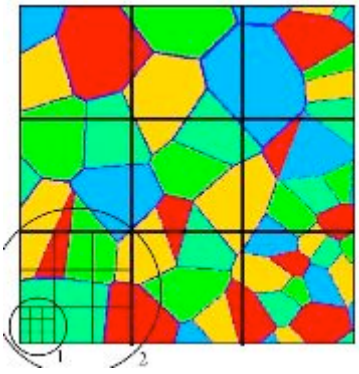

Figure 3: Vorni tessellation of a microstructure for the HMM.

7. FRAGMENTATION MODELING

Each material model has failure criteria that govern when it will no longer support a tensile load. In general, the criteria may be functions of the state variables including the temperature, equivalent plastic strain, the strain rate, and the stress. Most of the calculations we have performed to date have used the failure criterion in the Johnson-Cook plasticity model.

In a typical Lagrangian formulation, when a material in an element fails, the entire element fails and it is deleted from the calculation. Contact algorithms detect the new free surfaces generated by the element deletion and prevent their interpenetration.

Eulerian, and MMALE, formulations construct new material interfaces each time step based on the volume fractions of the material within an element and its neighbors. Since the mesh must cover the entire domain through which material may travel, elements cannot be selectively deleted since that would be equivalent to introducing holes in space. To introduce a new interface where material has failed, additional material must be introduced to make the interface reconstruction algorithm to construct an interface through the element. Since the new material must not introduce any strength into the element, we use a void material, equivalent to a vacuum. When the failed material is expanding, enough void material is introduced to preserve the density of the failed material. When the material fails in compression, a very small amount of void material is introduced to force the generation of a new free surface.

Deciding how to handle a material that fails, however, is only one aspect of modeling fragmentation. Consider, for example, a homogeneous cube that is pulled in tension uniformly in all three directions. The resulting stress and deformation of the cube are uniform, and therefore every point in the cube will fail at exactly the same time, reducing it to a gas. Real materials, however, don't behave this way, but fragment into particles that fit an exponential size distribution function. The fragmentation occurs because real materials aren't perfectly uniform, and some locations start to fail before others.

In the fragmentation model, the material parameters describing when a material fails are varied randomly over the mesh, making the material nonuniform. Becker has found that this approach produces realistic fragmentation that converges with mesh refinement. The high frequency component of the random field, however, decays as material is transported through the mesh, and at late times, the material is once again uniform. Benson and Vitali have addressed this issue by transporting the initial coordinates of the material, and interpolating the values of the material parameters from a mesh in the initial configuration.

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.